Crossovers due to anisotropy and disorder in quantum critical fluctuations.

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(Dated: March 29, 2017)

Abstract

Scaling relations are used to study cross-overs, due to anisotropic spin interactions or single ion anisotropy, and due to disorder, in the thermodynamics and correlation functions near quantum-critical transitions. The principal results are simple with a wide range of applications. The region of attraction to the stable anisotropic fixed point in the quantum-critical region is exponentially enhanced by the dynamical critical exponent z compared to the region of attraction to the fixed point in the quantum disordered region. The result implies that, even for small anisotropy, the region of attraction to the stable incommensurate Ising or planar metallic anti-ferromagnetic critical points, which belong to the universality class of the XY model with $z \to \infty$, covers the entire quantum-critical region. In crossovers due to disorder, the instability of the pure fixed point in the quantum disordered region is exponentially enhanced by z compared to that in the quantum-critical region. This result suggests that for some classes of disorder and for large enough z, one may find singularities in the correlations as a function of frequency and temperature down to very low temperatures even though the correlation length in space remains short range.

I. INTRODUCTION

Quasi-2D metals, in the vicinity of antiferromagnetic (AFM-ic) quantum critical points, exhibit singular fermi-liquid properties, such as linear in T contribution to the resistivity, and a $T \ln T$ contribution to the entropy [1] [2] [3] [4] characteristic of marginal Fermi-liquids [5]. Most of the theoretical work on AFM-ic critical points in metals is an extension of the Ginzburg-Landau-Wilson-Fisher (GLWF) theory of classical dynamical critical phenomena to quantum critical points. The starting Lagrangian for these works is isotropic in spin-space. The simple version of these theories are not consistent in problems in (2+1)D [6]. While such technical problems may have been solved [7], neither the old results nor the new appear to give results in agreement with experiments.

The AFM-ic ordering in these materials show them to be anisotropic in spin-space. Anisotropy is always a relevant parameter in classical phase transitions [8]; therefore it would not be surprising if the properties close enough to criticality are not of the isotropic model. But the observed anomalous properties occur over such a wide range of temperature that, unless the anisotropy is O(1), it is not possible to understand the region of attraction to the stable anisotropic critical point as given in the theory of classical phase transitions [8]. Anisotropy of O(1) is unreasonable. I therefore ask the question whether the effects of anisotropy get magnified in quantum-critical fluctuations compared to those in classical critical fluctuations. The answer to this questions turns out to be very simple and simply obtained. If the anisotropic problem has a critical exponent $z > 1$ the temperature scale to observe the critical fluctuations of the anisotropic critical point is exponentially enhanced by z compared to the classical criteria . No such expansion of scale occurs in the parameter p tuning the quantum transition.

Incommensurate Ising AFMs and commensurate or incommensurate planar AFMs in 2D map to the XY model for their critical properties [9], [4]. It is well known that this model does not belong to the universality class of the GLWF theories for classical phase transitions, which are in essence theories based on renormalization of spin-waves due to anharmonicity. The critical properties of the 2D-XY model, on the other hand occur through the proliferation of topological excitations in which the spin-waves serve only to determine their long-range interaction. Similarly, in the quantum 2D-XY model, supplemented by an appropriate dissipation (2D-DQXY model), the proliferation of topological defects, the 2D-

vortices and the warps - a variety of topological defects in time or instantons, determine the quantum-critical properties. The solution of this model [10–13] reveals that the dimensionless spatial correlation length ξ_r is proportional to the logarithm of the temporal correlation length ξ_τ, or $z = d \ln \xi_\tau / d \ln \xi_r$ is effectively ∞. Then a small anisotropy leads to a crossover from the properties of the isotropic model to the anisotropic model over almost the entire range of temperature. The critical fluctuations, in striking contrast to the GLWF - based theories, are products of a function of momentum and a function of frequency/temperature. The scattering of the Fermions by such fluctuations have the virtue of giving the observed marginal Fermi-liquid properties [4].

In several well studied quantum-critical experimental systems [14–16], the region of parameters in which singular properties as $T \to 0$ are observed is over a finite region of the parameter p. The spatial correlation length remains small while the temporal correlation length grows strongly as temperature decreases. A study of the cross-over due to disorder suggests that for certain classes of disorder, the anisotropy due to a large z is such as to keep the problem critical as a function of T while the spatial correlation remains short-ranged and the transition appears over a region in p with a small spatial correlation length.

II. SCALING FUNCTIONS FOR CROSS-OVER

Let us consider an isotropic Heisenberg model in a metal which has a quantum critical point as the dimensionless parameter p approaches the isotropic critical value p_i. Let us introduce a single-ion or exchange anisotropy. Just as in classical transitions, the flow-diagram is the same for either form of anisotropy. Let us consider the free-energy density $F(p, T, A)$, as a function of the departure from quantum criticality and as a function of the dimensionless anisotropy parameter A. A may be taken as the ratio of the anisotropic coupling energy to the isotropic coupling energy. Similarly T is dimensionless, being the ratio of the physical temperature to the ultra-violet cut-off energy, which is also similar to the isotropic coupling energy.

There is an unstable isotropic quantum critical point at $\delta p_i \equiv |p - p_i|/p_i = 0, T = 0$, and a stable anisotropic quantum-critical point at $\delta p_a \equiv |p - p_a|/p_a = 0, T = 0$. We wish to find the domain of attraction of the anisotropic critical point, as well as an estimate of $(p_a - p_i)$.

I will assume that scaling holds for both the isotropic and the anisotropic quantum-critical

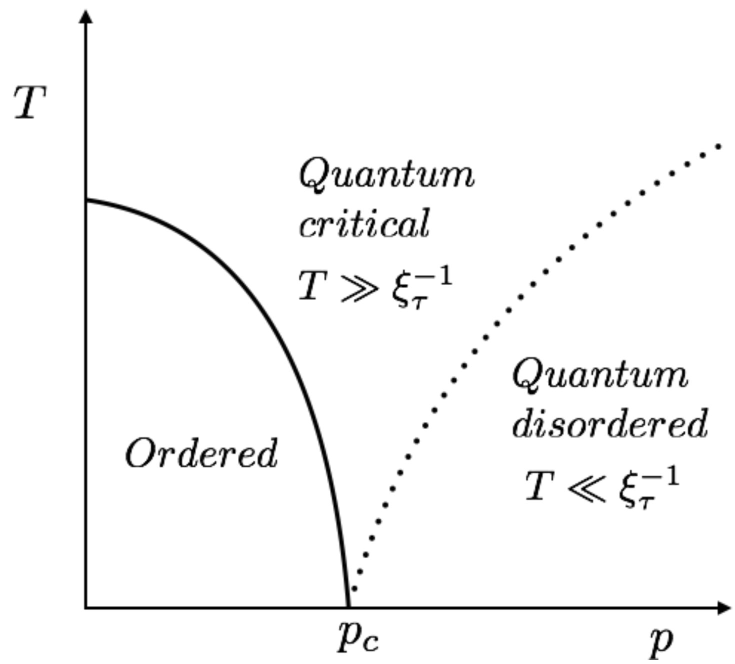

Figure 1. Typical phase diagram for a transition with a quantum-critical point as a function of a parameter p, showing the quantum-disordered region in which the characteristic energy of fluctuations is much larger than the temperature and the quantum critical region in which the reverse is true.

point under discussion. The justification for this is given at the end of the paper. Let us start from the isotropic critical point. On a length scale ℓ, the scaling for the action, which is the simple generalization to quantum-critical phenomena of the form for classical critical phenomena is, see for example [17, 18],

$$S(p,T,A) = F(p,T,A)/k_BT \propto \ell^{-(d+z_i)} f(\delta p_i \ell^{y_{pi}}, T\ell^{z_i}, A\ell^{y_{A_i}}). \tag{1}$$

The singularities in the specific heat coefficient C_v/T and the p-susceptibility χ_p are given by the second derivatives of F with respect to T and p respectively, with the other held constant. Also introduced are the dynamical critical exponent z_i for the isotropic problem and the renormalization group eigenvalues $y_{pi} = 1/\nu_i$ and y_{Ai} for the operators p and A, respectively. $y_{Ai} > 0$, as for a relevant scaling operator.

Now we use the scaling hypothesis near criticality, separately for the two fluctuation regions in the characteristic phase diagram Fig. (1) for quantum transitions. In the so-called quantum fluctuation region, the infra-red cut off scale for energies is set by k_BT,

while in quantum-disordered regime, the characteristic energies are much larger than $k_B T$ [19]. For $T\ell^{z_i} << 1$, we can replace the dependence of f on $T\ell^{z_i}$ by 1, and get scaling in the p-direction:

$$S(p,T,A) \propto \delta p_i^{(d+z_i)\nu_i} f_p(A/\delta p_i^{\nu_i y_{Ai}}). \tag{2}$$

This gives the cross-over at $\delta p_{iX} \approx A^{1/\phi_i}; \phi_i \equiv \nu_i y_{Ai}$. For $\delta p_i \lesssim \delta_{Xi}$, the flow is towards the anisotropic critical point. This is completely akin to cross-over in classical problems in which δp_i is the dimensionless deviation from the critical temperature [17].

For classical transitions in models with n component spins and in (4-ϵ) dimensions, the cross-over exponent calculated to $O(\epsilon)$ is [8],

$$\phi_i = 1 + \frac{n\epsilon}{2(n+8)}. \tag{3}$$

We may safely take $\phi_i \approx 1$ for our problems.

In the quantum-fluctuation regime, i.e. $T\ell^{z_i} >> 1$, and $z_i > 1, \delta p_i \ell^{1/\nu_i} \to 0$ and we can replace dependence of this quantity in f by 1, to get scaling in the T-direction:

$$S(p,T,A) = T^{(d+z_i)/z_i} f_T(A/T^{(y_{A_i}/z_i)}). \tag{4}$$

This shows that the influence of the isotropic critical point at $\delta p_i = 0$ disappears and the flow is towards the anisotropic critical point at $\delta p_a = 0$ for $T \lesssim T_{iX} \approx A^{(z_i\nu_i)/\phi_i}$. A $z_i\nu_i > 1$ reduces the region of cross-over in temperature relative to that in the control parameter δp_i for the quantum transition.

Let us consider the scaling around the anisotropic problem and treat $\overline{A}$, the complement of A, $(A+\overline{A} = 1)$, as the *irrelevant* variable. $\overline{A}$ is an operator with scaling eigenvalue $y_{\overline{A}a} \approx -1$ around the anisotropic critical point. Let ν_a and z_a be the corresponding correlation length and dynamical exponents, respectively. As already mentioned, the quantum critical point shifts from p_i for the isotropic case to p_a.

One finds by the same procedure as above that the *region of attraction* of the anisotropic critical point around $\delta p_a = 0$ extends to

$$\delta_{Xa} \approx \overline{A}^{(-1/|\phi_a|)},\ \phi_a \equiv \nu_a |y_{Aa}|\ for\ T << \delta p_a^{-z_a\nu_a}, \tag{5}$$

$$T_{Xa} \approx \overline{A}^{-(z_a\nu_a)/|\phi_a|},\ for\ T >> \delta p_a^{-z_a\nu_a}. \tag{6}$$

It is only beyond δ_{Xa} and T_{Xa} that one notices the isotropic critical point. The isotropic fixed point is exponentially more irrelevant in the temperature direction as z_a increases. For

$(z_a\nu_a)/|y_{Aa}| >> 1$, the region of influence of the anisotropic critical point extends over the entire temperature range, of $O(1)$ for any range of $\overline{A}$.

The same conclusions can be reached about the correlation function $C(r,\tau,T,A)$ as a function of the order parameter separated in space by r and in imaginary time by τ. Putting the scaling near the isotropic and anisotropic critical points together, the conclusion is that in the $p-$direction, the crossover is similar to the crossover in temperature of the classical problem. On the other hand, in the temperature direction, $z_a >> z_i$ leads to properties which are close to that of the anisotropic critical point over the whole range. In fact for $z_a \to \infty$ as for the 2D-DQXY model, there is no region of applicability of the isotropic model along the temperature axis for p close to the critical value, for even very small anisotropy.

We can also get an estimate of the change in the critical value of p due to the crossover to the anisotropic critical point through scaling arguments. Consider the p-susceptibility obtained from free-energy (2) from the quantum-fluctuation side. It may be written as

$$\chi_p(p,T,A) \propto \delta p_i^{-\gamma_i} f_p(A\delta p_i^{-\phi_{ip}});\ \gamma_i \equiv 2-(d+z_i)\nu_i;\ \phi_{ip} \equiv \nu_i y_{Ai}. \tag{7}$$

We can equally write this as

$$\chi_p(p,T,A) \propto A^{-\gamma_i/\phi_{ip}} \tilde{f}_p(\delta p_i A^{-1/\phi_{ip}}). \tag{8}$$

We expect that the actual singularity in $\chi_p(p,T,A)$ must be of the form $\chi_0(A)\delta p_a^{-\gamma_a}$. This can be so only if

$$\tilde{f}_p(\delta p_i A^{-1/\phi_{ip}}) \propto (\delta p_i A^{-1/\phi_{ip}} - c)^{-\gamma_a} = A^{\gamma_a/\phi_{ip}}(\delta p_i - cA^{1/\phi_{ip}})^{-\gamma_a}, \tag{9}$$

where c is a constant. So, the shift in the critical point, $\delta p_i - \delta p_a = cA^{1/\phi_{ip}}$. This is the same as the change in transition point and amplitude for the case of classical transitions as a function of temperature.

It also follows, conversely from the above, that for any relevant operator about a quantum-critical point with a large dynamical critical exponent z, the region for small $|p-p_c|$ below which the flow is away from the critical point is similar to that in the classical transition. But the region of temperature below which the flow is away from the critical point is exponentially narrowed and for large enough z may never be visible.

Applications:

As one example, let us consider the 2D antiferromagnetic Heisenberg model as for the 1/2 filled (insulating) layered cuprates, which is argued [19] to be isotropic to a first approximation with a small spin anisotropy and a larger inter-planar coupling. The theory for the isotropic model, as equivalent to the non-linear quantum sigma model [19], has a transition at $T = 0$, but the 3 dimensional ordering occurs in all cuprates with spins in the plane in the $(1, 1)$ (or equivalent directions.) We might suspect that the purely 2 dimensional model flows to a quantum XY model with four-fold anisotropy. However, the isotropic model as well as the XY model in this case have a dynamical exponent 1. No extended region in flow in the quantum-critical region towards the XY critical point is therefore to be expected. The temperature dependence in the correlation function between the temperatures of the order of the exchange energy (about 10^3 K) and the 3D ordering temperature (about 250 K) is properly explained [19] without considering flow to the anisotropic critical point.

It is remarkable how the quantum critical fluctuations change on driving the AFM-ic transition to $T = 0$ with a small doping into the metallic state in the same compounds. The measured critical fluctuation spectra $Im\chi(\mathbf{q}, \omega, T)$, above the small temperature of a spin-glass phase, over a wide temperature and frequency ω shows proportionality to $\tanh(\omega/2T)$ form and a magnetic correlation length which is nearly independent of both ω and T [20–22]. These are the properties of the 2D-DQXY model [10–12], where the correlation function is found to be product of a function of momentum and a function of ω/T of this form. Properties consistent with such behavior are found by inelastic neutron scattering in $La_{2-x}Sr_xCuO_4, La_{2-x}Ba_xCuO_4$, and in $YBa_2Cu_3O_{6.4+x}$ for small x [20–22], and fitted long ago to the phenomenological critical spectra suggested for a marginal Fermi-liquid. It is therefore suggested that doping introduces dissipation in the model so that even with small anisotropy, the system is driven to the properties of the DQXY model. The flow due to disorder considered in the next section may be relevant to the fluctuations above the spin-glass phase.

As mentioned earlier, quasi-2D Fe-based AFM-ic compounds and several heavy-fermion compounds in their quantum-critical region, also display thermodynamic and transport properties of a marginal Fermi-liquid. The rather limited inelastic neutron scattering measurements [23, 24] exploring quantum-critical fluctuations on them can be fitted [25] to the fluctuation spectra of the 2D-DQXY model. An important prediction for these compounds is that the single-particle scattering rate should be proportional to $max(\omega, T)$ over the whole

fermi-surface. A linear single-particle scattering rate has been observed in ARPES experiments in a heavy-fermion compound [26] in one direction but the angular dependence has not yet been measured. The fact that the low temperature specific heat appears to be $\propto T \ln T$ without a noticeable residual T component in the quantum-critical region of a Fe-based AFM/superconductors [27] does however suggest that the entire Fermi-surface is hot. Complete ARPES experiments for the heavy-fermion and other AFMs near quantum criticality are suggested to settle this very important question.

III. CRITERIA FOR RELEVANCE OF DISORDER FOR QUANTUM CRITICAL POINTS

Suppose the quantum critical point p_c is a function of disorder. The analogous classical problem is the problem in which the transition temperature varies spatially depending on disorder, which was formulated by Harris [28].) The correlation functions appear, as for the classical phase transitions, strongly dependent on the nature of disorder [28, 29]. Consider first, disorder $D(\mathbf{r},\mathbf{r}') = (\Delta D)^2\delta\delta(\mathbf{r}-\mathbf{r}')$, with short-range correlations compared to ξ_r, with root-mean-square value $(\delta D)^2$. The disorder is fixed in (imaginary) time τ. The variance disorder in a spatial length scale ℓ_r and temporal length scale ℓ_τ is .

$$\Big(\int \frac{d\tau}{\ell_\tau}\frac{d\tau'}{\ell_\tau}\frac{d^dr}{\ell_r}\frac{d^dr'}{\ell_r}D(\mathbf{r},\mathbf{r}')\Big)^{1/2} = \delta D(\ell_r)^{-d/2}\ell_{tau}^{-1} \tag{10}$$

Instead of $A\ell_r^{\phi_A}$ in (1), let us use (10), which provides the magnitude and renormalization eigenvalue of disorder to estimate its relevance. Using $\ell_{tau} \propto \ell_r^z$, one finds that the root mean square disorder grows under scaling near criticality $\delta p \to 0$, for $T\ell_\tau \to 0$ if

$$(d/2+z)\nu - 1 < 0. \tag{11}$$

This generalizes the Harris criteria $d\nu/2 - 1 < 0$ for the relevance of disorder in classical problems to quantum criticality.

Let us look at the crossover due to disorder in the temperature direction, meaning $\delta p\ell_r^{1/\nu} \to 0$. Now the criteria for relevance of disorder is

$$T^{d/2z} \gtrsim 1. \tag{12}$$

These criteria can be used generally. For the 2D-DQXY model and for the relevant change in variable of approaching the quantum-critical point [13], $z\nu_p \approx 1/2$, while $\nu_p = 0$, i.e.

$\xi_r \propto \ln(p-p_c)$ and $z \to \infty$. Then disorder is relevant in the $p-$ direction while it is marginal in the $T-$ direction. Scaling arguments do not tell if it is marginally irrelevant or relevant. In either case, the dependence is weak compared to that in the $p-$direction.

What are the properties of the system if disorder is a relevant perturbation? Even for the classical problems, the answer to this question is not completely clear. For weak and weakly correlated disorder discussed above, the answer from ϵ-expansions is that the disorder stable transition is also a sharp transition [29, 30]. This is in contrast with experiments which often show quite rounded transitions in disordered samples. So one must investigate other classes of disorder.

The situation is quite different for disorder with correlations with long tails, or disorder in which there is a random spatial distribution of clusters, with similar coupling constants inside the cluster. In the latter case, which may be considered the opposite limit of the weak Gaussian correlated disorder, Δp_c does not depend on the correlation length; it only depends on the root mean-square of the bare coupling constant which is of $O(p_c)$ itself. Disorder then is always strongly relevant and the pure classical transition is eliminated. The correlation length ξ_r will be of the size of the cluster in each cluster acting as a domain, with mean-square fluctuations in ξ_r are of the order of the fluctuations of the cluster size.

If in the pure limit, ν_p is very small or 0, i.e. $\xi_r \propto \log|p-p_c|$ and p_c is disordered, the spatial correlation length is of the order only of a lattice constant at a distance $|p-p_c|/p_c$ of $O(1/10)$. At that point, impurity cluster of size of the order of a lattice constant fluctuate only weakly correlated with the others and the correlation length remains of that order as $T \to 0$. But the temporal correlation length goes as $\xi_\tau \propto (|p-p_c|/p_c)^{-\nu}$, $\nu \approx 1/2$. This is sufficiently large that the disorder may be irrelevant or only weakly relevant in the T-direction. One can thereby have a sharp and growing temperature dependence of ξ_τ with ξ_r remaining of the order of a lattice constant.

There can be range of correlations of disorder between the two limits discussed above. Where the boundary to the two classes of disorder induced critical points falls is, as in classical phase transitions, not clear. What is interesting is that in the class of disorder in which the classical phase transitions show a smeared out transition in a range around the pure T_c, with short correlation lengths and with corresponding smeared out dynamics, a quantum phase transition can in principle show a temporally sharp transition for $T \to 0$, ocurring in a range of $(p-p_c)$ with short-range spatial correlations.

Applications:

There is a long history of disordered heavy-fermion compounds [14–16] which show no spatial correlations while the temporal correlations measured in μSR and NMR experiments as well as by neutron scattering show divergences down to low temperature over a range of variations in composition. The ideas that this may be due to random single-site parameters is not tenable [31]. These would be candidates for the anisotropic disordered criticality if z in the model appropriate for them were sufficiently high. But, not enough information to determine z and ν is available. Enough information, from magnetization and correlation functions through inelastic scattering, is however available on the transition metal compound YFe_2Al_{10} to be reasonably certain that it belongs to the ferromagnetic 2D-XY class of models [32]. The spatial correlations are quite local while the temporal correlations show criticality. It should be noted that in the pure system, the spatial correlation in the pure model is proportional to the logarithm of the temporal correlation length. The correlation length even in the pure system is then on the scale of a lattice constant except exponentially close to the critical point. So even moderate disorder is likely to lead to a non-critical correlation length while the correlation time can grow to large values.

Concluding Remarks

The results obtained here assume that scaling holds for the problems under consideration and that it by itself can give the correct answers. In the quantum-critical theories based on the Ginzburg-Landau-Wilson method, this is not true for $d + z \geqslant 4$. Such theories should work for the quantum-critical fluctuations of the (2+1)D XY model in which $z = 1$, and which are equivalent to the classical 3D XY model. So, for this model, there is no difficulty. On the other hand for the Dissipative quantum XY model, $z \to \infty$, and this behavior of z has played a crucial role above in the application of the theory to experiments. But this model does not belong to the Ginzburg-Landau universality class and the spin-wave arguments used for the upper critical dimension cannot be applied. Moreover, the analytic solution of the model by RG (Ref. (12)) does yield scaling and defines ξ_r and ξ_τ; and the Monte-Carlo calculations on it (Ref. (11) and (13)) are consistent with the RG results. The theory also gives ω/T scaling explicitly, which is unlike the Ginzburg-Landau-Wilson type theories above the upper critical dimension.

The other issue is about the variation of non-universal amplitudes in determining cross-overs. For strong cross-overs as obtained for large z, this should not be important.

Application of the ideas of quantum-criticality to actual experimental systems requires considerations of crossover, such as have been undertaken here. Further work, especially Monte-Carlo calculations is urged for both crossovers due to anisotropy and varieties of disorder.

I wish to thank Alexei Tsvelik for a discussion about the influence of disorder on quantum critical phenomena.

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